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Challenges in bimetallic multilayer structure formation:

Pt growth on Cu monolayers on Ru(0001)

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In a joint experimental and theoretical study, we investigated the formation and morphology of PtCu/Ru(0001) bimetallic surfaces grown at room and higher temperatures under UHV conditions. We obtained the PtCu/Ru(0001) surfaces by deposition of Pt atoms on a previously created Cu/Ru(0001) structure which includes only one Cu monolayer. Bimetallic surfaces obtained at different Pt coverages are investigated using STM imaging, revealing the existence of reconstruction lines and Cu islands. Although primary created Cu islands continue growing in size by increasing Pt coverage, a continuous formation of new Cu islands is observed. This leads to an atypical exponential increase of the island density as well as to an atypical behavior of the average number of atoms per island for low Pt coverages. Although coalescence of the islands is observed for high Pt coverages, the island density remains almost constant at that regime. In order to understand the trends observed in the experiments, we study the stability of these surfaces, atom adsorption, and adatom diffusion using periodic density functional theory calculations. On the basis of the experimental observations and the first-principles calculations, we suggest a model that includes exchange of Pt adatoms with Cu surface atoms, Pt and Cu adatom diffusion, and attractive (repulsive) interactions between Cu (Pt) adatoms with substitutional Pt surface atoms, which explains the main trends in island formation and growth observed in the experiment.

Keywords: Bimetallic surfaces, exchange, nucleation and growth, Pt, Cu/Ru(0001), STM, DFT

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